CONF-840202--17

DE84 007557

# PREPAR - A USER-FRIENDLY PREPROCESSOR TO CREATE AIRDOS-EPA INPUT DATA SETS

Andrea L. Sjoreen
Computer Sciences

Charles W. Miller
Health and Safety Division

Oak Ridge National Laboratory*
Union Carbide Corporation, Nuclear Division
Oak Ridge, Tennessee 37830

Christopher B. Nelson
U.S. Environmental Protection Agency
Washington, D.C.

By acceptance of this article, the publisher or recipient acknowledges the U.S. Government's right to retain a nonexclusive, royalty-free license in and to any copyright covering the article.

**DISCLAIMER**

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MASTER

*Operated by Union Carbide Corporation under contract W-7405-eng-26 with the U.S. Department of Energy.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

# PREPAR - A USER-FRIENDLY PREPROCESSOR TO CREATE AIRDOS-EPA INPUT DATA SETS

Andrea L. Sjoreen and Charles W. Miller
Oak Ridge National Laboratory
Oak Ridge, Tennessee

Christopher B. Nelson
U.S. Environmental Protection Agency
Washington, D.C.

## ABSTRACT

PREPAR is a FORTRAN program designed to simplify the preparation of input for the AIRDOS-EPA computer code. PREPAR was designed to provide a method for data entry that is both logical and flexible. It also provides default values for all variables, so the user needs only to enter those data for which the defaults should be changed. Data are entered either unformatted or via a user-selected format. A separate file of the nuclide-specific data needed by AIRDOS-EPA is read by PREPAR. Two utility programs, EXTRAC and RADLST, were written to create and list this file. PREPAR writes the file needed to run AIRDOS-EPA and writes a listing of that file.

## INTRODUCTION

PREPAR is a FORTRAN program designed to simplify the preparation of the input file for AIRDOS-EPA (Moore et al. 1979). Preparing the input for AIRDOS-EPA can be a cumbersome and confusing task. PREPAR was designed to provide a method for data entry that is both logical and flexible. It also provides default values for all variables, so the user needs only to enter that data for which the defaults should be changed.

The AIRDOS-EPA computer code was written for the U. S. Environmental Protection Agency (EPA) to assist them in regulating nuclear effluents covered by the Clean Air Act amendments of 1977. This code was subsequently used by EPA as a part of the process for setting radionuclide emission standards for both U. S. Nuclear Regulatory Commission licensed facilities and U. S. Department of Energy facilities (USEPA 1983). AIRDOS-EPA employs a Gaussian plume atmospheric dispersion model and an implementation of the U.S. Nuclear Regulatory Commission (NRC) Regulatory Guide

1.109 (USNRC 1977) terrestrial transport models to calculate dispersion of radionuclide pollutants from point or area source releases through the surrounding atmospheric and terrestrial environment. The code uses meteorological and agricultural information to calculate concentrations in air, water, surface soil, beef, milk, and vegetables at several downwind receptor sites. Exposure to individuals or populations from immersion in air and water; standing on the ground surface; ingestion of beef, milk, and vegetables; and inhalation of air are calculated from the environmental concentrations using various parameters and scenarios pertaining to human activities and intake rates. AIRDOS-EPA has been widely used in radiological assessments, e.g., Cotter et al. (1980) and Baes and Sharp (1981).

AIRDOS-EPA may also convert exposures into radiological doses. However, this option is generally not used by EPA. Instead, the computer code DARTAB (Begovich et al. 1981) combines dose and risk factors for a particular nuclide with exposure and intake rate estimates from AIRDOS-EPA. The dosimetric data is read from a file compiled through numerous runs of the RADRISK computer code (Dunning, Leggett, and Yalcintas 1980). DARTAB tabulates doses and health risks by cancer, exposure pathway, or nuclide.

The program EXTRAC, written to provide dosimetric data for PREPAR, performs some of the computations done by DARTAB. Because of this, in some cases, the same results may be obtained by running PREPAR and AIRDOS-EPA as by running AIRDOS-EPA and DARTAB. However, AIRDOS-EPA does not produce the same set of formatted tables as does DARTAB.

This paper discusses the PREPAR input and output, the calculations done in PREPAR, and the program EXTRAC. A complete user's manual for PREPAR and EXTRAC is being written (Sjoreen and Miller, in press).

## DATA INPUT FOR PREPAR

PREPAR has been designed to require the mimimum possible amount of input. PREPAR provides default values for all the data needed by AIRDOS-EPA. The PREPAR documentation lists these default values. To run PREPAR, you must inspect the default values for the data and determine which ones need to be changed for your application and only those values are entered. For example, default values are available for all radionuclide dosimetric and physical data, so that only the radionuclide name and release rate need to be entered in most cases. Of course, any of this default data may be overridden if necessary.

Along with the user prepared data, two files are needed by PREPAR. A file of wind data in STAR format is needed if the AIRDOS-EPA wind arrays are not available. The file of dosemetric data is written by EXTRAC and is created from TEMPLT, a file created for this system, and the DARTAB-RADRISK data base (Begovich et al. 1981). TEMPLT was

created by concatenating element-specific data onto the radionuclide-specific data needed for decay and external dose calculations. The element-specific data were primarily taken from Baes et al. (1983). The removal rate constant for physical loss by weathering is from Miller and Hoffman (1982). The environmental decay constants for land and water surfaces were arbitrarily set to zero. The radionuclide-specific data in TEMPLT were taken from Kocher (1981), and include photon dose-rate factors for the body surface for air immersion, water immersion, and ground-surface exposure.

## CALCULATIONS DONE IN PREPAR

### Wind Data Computations

PREPAR allows two methods for entry of the wind data needed by AIRDOS-EPA. These data are the wind direction and stability class frequencies and the arithmetic- and harmonic-average wind speeds. If a file of these data is available from a previous run of AIRDOS-EPA, PREPAR will read that data directly. If data are not available in the AIRDOS-EPA format, PREPAR will compute these data from the joint freguency distribution of wind direction, wind speed class, and stability catagory which is in the format generated by the National Climatic Center's STAR program (e.g., Busse and Zimmerman 1973).

### Deposition and Gravitation Fall Velocities

In the absence of precipitation, particles and reactive gases may deposit on various surfaces via impingement, electrostatic interactions, chemical reactions, and other processes. In AIRDOS-EPA, these dry deposition processes are parameterized in terms of a dry deposition velocity, $V_d$ (m/s). This parameter is defined as the ratio between the rate at which material is being deposited on the surface of the earth (flux density) and the air concentration measured at some reference height, usually 1 m, above the earth. Note that $V_d$ is merely a proportionality factor even though it has the units of velocity.

PREPAR allows input of $V_d$ and $V_g$, the gravitational fall velocity. However, these variables may be computed within PREPAR for particles. The computations are done assuming a reference height of 1 m using the model of Sehmel and Hodgson (1975, 1980). These calculations are performed using algorithms developed by Nelson (1982). For gases, the gravitational fall velocity is set to zero and the deposition velocity is 0.0 cm/s for unreactive gases, 0.018 cm/s for relatively unreactive gases, and 3.5 cm/s for reactive gases (Moore et al. 1979).

For the assessment of inhalation doses, the activity median aerodyuamic diameter (AMAD) is required rather than

the physical diameter of the particle. The aerodynamic diameter of a particle is the diameter of an equivalent unit density sphere with the same settling velocity as the particle itself (Morrow et al. 1966). The AMAD of an aerosol is the particle diameter associated with the median of the distribution of activity against aerodynamic diameter. A default value of 1 gm/cm$^3$ is used for the particle density in PREPAR. Either a value for the physical particle diameter (PARDIA) or a value for the AMAD should be entered for each nuclide in PREPAR. The default value of AMAD and PARDIA is 1 ;m. If only PARDIA is entered, AMAD is calculated by multiplying PARDIA by the square root of the particle density. If only AMAD is entered, PARDIA is calculated by dividing AMAD by the square root of the particle density. Note that if the default density is not overridden, PARDIA and AMAD will be equal. If the default density is overridden and no AMAD or a PARDIA are entered, a warning message will be written. Of course, the user may input both PARDIA and AMAD, in which case no calculations are made.

Scavenging Coeffient

In the presence of precipitation, radionuclides may be removed from a plume primarily by being incorporated into the precipitation as it is formed (rainout), or by being swept out of the air by the precipitation as it falls (washout) (Engelmann 1968). In AIRDOS-EPA, both these processes are parameterized in terms of SC, the scavenging rate. It is assumed that the scavenging process is irreversible.

The values of SC in PREPAR are calculated using algorithms developed for the ATM code (Culkowski and Patterson 1976). Particulate SC's are calculated on the basis of Fig. 5-9 in Meteorology and Atomic Energy - 1968 (Engelmann 1968). A set of SC's as a function of particle diameter, particle density, and rainfall rate has been adopted from the ATM code. Values of SC for gases and very small particles that are unaffected by electrical charges and impaction are calculated on the basis of the Kelkan-Hanford curve of Fig. 5-11 in Meteorology and Atomic Energy - 1968 (Engelmann 1968),

$$SC = 5.55 \times 10^{-4} R^{0.6} y \qquad (1)$$

where R is the rainfall rate when it is raining (mm/h) and y is the gas diffusivity (m$^2$/s).

PREPAR uses a default value of y of 0.0001 m$^2$/s. The default value of R is 5 mm/h (Slinn 1977). Both y and R may be entered by the user. Alternatively, values of SC may be entered directly. One source of values for SC is empirical measurements of washout ratios for various depositing substances and types of precipitation and precipitation systems; e.g., Semonin and Beadle (1977).

## Unit Conversion and Miscellaneous Computations

Several miscellaneous computations are done in PREPAR. For example, the ambient air temperature is entered in Celsius and converted to Kelvin as required by AIRDOS-EPA. If the user choses to enter the nuclide release in Becquerels, the release is converted to Curies. The breathing rate of man is entered in $m^3/y$ and converted to $cm^3/h$. The total amounts of milk, beef, and vegetables produced at an individual's location, produced in the entire assessment area excluding the individual's location, and produced external to the assessment area are entered to PREPAR to compute the fractions produced locally and the minimum fraction imported in each catagory. The external ground surface dose conversion factor is multiplied by an input factor to adjust for ground surface roughness.

## OUTPUT FROM PREPAR

The main purpose for running PREPAR is to create a data file that can be used as the input file for AIRDOS-EPA. This file can be edited by the user with any standard text editor.

The listing that is written by PREPAR includes all the data in the AIRDOS-EPA input file and of any data that were entered to PREPAR that are not passed to AIRDOS-EPA. An executive summary of this data is included as the last two pages of the output. This listing can be used instead of the AIRDOS-EPA listing of input data and is more concise and better organized than that listing. Data that undergo unit conversion in PREPAR are listed in both input and output units. If STAR wind data are entered, those data are listed with the computed AIRDOS-EPA wind arrays. All user options are listed, including both the entered value of the option and the meaning of that value. Warning messages are printed at the beginning of the PREPAR report for any data entered that seem inconsistent or will be disallowed by AIRDOS-EPA.

## EXTRAC

The purpose of the program EXTRAC is to extract the dose factors for ingestion and inhalation dose from the DARTAB-RADRISK data base, compute ratios for converting body surface doses to organ doses (FROG values), and to merge these data with the other element- and radionuclide-specific data.

The user input to EXTRAC allows an expansion of the capabilities of AIRDOS-EPA. Low-LET or high-LET dose factors, dose equivalent factors, or risk equivalent factors may be selected from the data base. EXTRAC will compute a dose factor which is a composite or weighted sum from organ names and weights requested. Organ names other than those in the default AIRDOS-EPA list may be used. The default

values of the input are such that the default output will consist of the dose equivalent factors for the 11 standard AIRDOS-EPA organ names selected for a time of 70 years and computed with a quality factor of 20.

This program extracts dose factors for all nuclides in RADRISK. If a nuclide had more than one set of available factors, one set is selected as the default to be used in PREPAR, and the index of this set is written to the output file. If no factors of the selected type are found for a nuclide, the dose factors are set to zero and the number of sets of factors for the nuclide is written as zero. PREPAR tests for this zero value and writes a warning message for each such nuclide.

The computations done by EXTRAC consist of performing unit conversions and computing FROG values. The FROG values are computed as the organ specific dose factors for air immersion divided by the value of the body surface dose converison factor for submersion in air for the nuclide. If high-LET dose factors are selected, the FROG values are set to zero.

The output of EXTRAC is a formatted file which is used as input to PREPAR. If the user wishes to alter any of the values in this file, it may be edited with a text editor. EXTRAC prints warning messages but does not print the extracted dose factors. RADLST produces a listing of the factors from the output of EXTRAC.

## SUMMARY

The program PREPAR will simplify the preparation of AIRDOS-EPA input data sets, and the program EXTRAC increases the types of dose calculations possible in AIRDOS-EPA. PREPAR allows a minimum of user input with a maximum of flexiblity in the input method. The PREPAR user must be familiar with AIRDOS-EPA variables names and be somewhat familiar with FORTRAN input types. The AIRDOS-EPA user should be familiar with these in any case. The program EXTRAC is designed to require very little user input unless very special types of dose factors are required. RADLST produces a concise listing of the dosimetric data needed in AIRDOS-EPA for all DARTAB-RADRISK nuclides.

## REFERENCES

Begovich, C. L., K. F. Eckerman, E. C. Schlatter, S. Y. Ohr, and R.O. Chester. 1981. DARTAB: A Program to Combine Airborne Radionuclide Environmental Exposure Data with Dosemetric and Health Effects Data to Generate Tabulations of Predicted Health Effects. ORNL-5692.

Baes, C. F., III and R .D. Sharp. 1981. A Directory of Parameters used in a Series of Assessment Applications of the AIRDOS-EPA and DARTAB Computer Codes. ORNL-5710.

Baes, C. F., III, R. D. Sharp, A. L. Sjoreen, and R. W. Shor. (in press). A Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides Through Agriculture. ORNL-5786.

Businger, J. R., J. C. Wyngaard, Y. Izumi, and E. F. Bradley. 1971. Flux-profile relationships in the atmospheric surface layer. J. Atmos. Sciences 28:181-189.

Busse, A. D., and J. R. Zimmerman. 1973. User's Guide for the Climatological Dispersion Model. EPA-RA-73-024 (NTIS PB 227346/AS).

Cotter, S. J., C. W. Miller, R. E. Moore, and C. A. Little. 1980. Estimates of Dose Due to Noble Gas Releases from the Three Mile Island Incident Using the AIRDOS-EPA Computer Code. ORNL-5649.

Culkowski, W. M., and M .R. Patterson. 1976. A Comprehensive Atmospheric Transport and Diffusion Model. ORNL/NSF/EATC-17.

Dunning, D. E., Jr., R. W. Leggett, and M. G. Yalcinats. 1980. A Combined Methodology for Estimating Dose Rates and Health Effects from Radioactive Pollutants. ORNL/TM-7105.

Engelmann, R. J. 1968. The calculation of precipitation scavenging. pp. 208-221. In D. Slade(ed.), Meteorology and Atomic Energy - 1968. USAEC TID-24190.

Kocher, D. C. 1981. Dose-Rate Conversion Factors for External Exposure to Photons and Electrons. NUREG/CR-1918, ORNL/NUREG-79.

Miller, C. W., and F. O. Hoffman. 1982. An analysis of reported values of the environmental half-time for radionuclides deposited on the surfaces of vegetation. pp. 313-328. In Environmental Migration of Long-Lived Radionuclides. IAEA-SM-257/63.

Moore, R. E., C. F. Baes III, L. M. McDowell-Boyer, A. P. Watson, F. O. Hoffman, J. C. Pleasant, and C. W. Miller. 1979. AIRDOS-EPA: A Computerized Methodology for Estimating Environmental Concentrations and Dose to Man from Airborne Releases of Radionuclides. ORNL-5532.

Morrow, P. E. (Chm.), D. V. Bates, B. R. Fish, T. F. Hatch, and T. T. Mercer, Task Group on Lung Dynamics. 1966. Deposition and retention models for internal dosimetry of the human respiratory tract. Health Phys., 12:173-207.

Nelson, C. B. 1982. Personal communication to C. W. Miller.

Sehmel, G. A., and W. H. Hodgson. 1975. Predicted dry deposition velocities. pp. 399-422. In Proceedings of the Atmosphere Surface Exchange of Particulate and Gaseous Pollutants - 1974 Symposium. CONF-740921.

Sehmel, G. A., and W. H. Hodsgon. 1980. A model for predicting dry deposition of particles and gases to environmental surfaces. pp. 218-230. In Implications of the Clean Air Amendments of 1977 and of Energy Considerations for Air Pollution Control. American Institute of Chemical Engineers Symposium Series 196, Volume 76.

Semonin, R. G., and R. W. Beadle (eds.). 1977. Precipitation Scavenging (1974), Proceedings of a symposium held at Champaign, Illinois, October 14-18, 1974. CONF-741003.

Sjoreen, A. L. and C. W. Miller. (in press). PREPAR - A User-Friendly Preprocessor for AIRDOS-EPA. ORNL-5952.

Slinn, W. G. N. 1977. Precipitation scavenging: some problems, approximate solutions, and suggestions for future research. pp. 1-60. In R. G. Semonin and R. W. Beadle (eds.), Precipitation Scavenging (1974), Proceedings of a symposium held at Champaign, Illinois, October 14-18,1974. CONF-741003.

U. S. Environmental Protection Agency. 1983. 40 CFR Part 61, National emmission standards for hazardous air pollutants, Proposed standards for radionuclides. Federal Register, April 6, 1983.

U. S. Nuclear Regulatory Commission. 1977. Calculation of Annual Doses to Man from Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50, Appendix I. Regulatory Guide 1.109, Revision 1. Office of Standards Development.